

# Template $\text{\LaTeX}$ Wiki von BAzubis für BAzubis

## Projektarbeit 1 (T2\_2000)

im Rahmen der Prüfung zum  
**Bachelor of Science (B.Sc.)**

des Studienganges Angewandte Informatik  
an der Dualen Hochschule Baden-Württemberg Karlsruhe

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**-Sperrvermerk-**

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Ausbildungsfirma:	SAP SE Dietmar-Hopp-Allee 16 69190 Walldorf, Deutschland
Betreuer der Ausbildungsfirma:	B-Vorname B-Nachname
Gutachter der Dualen Hochschule:	DH-Vorname DH-Nachname

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SAP SE  
Dietmar-Hopp-Allee 16  
69190 Walldorf, Deutschland

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Try to include in this abstract the main question of your work, the methods you used or the main results of your work.

## **Abstract**

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Versuche in das Abstract folgende Punkte aufzunehmen: Fragestellung der Arbeit, methodische Vorgehensweise oder die Hauptergebnisse deiner Arbeit.

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# List of abbreviations

<b>DE</b>	Differential Equation
<b>DFT</b>	Discrete Fourier Transform
<b>FEM</b>	Finite Element Method
<b>FT</b>	Fourier Transform
<b>FFT</b>	Fast Fourier Transform
<b>IDFT</b>	Inverse Discrete Fourier Transform
<b>IFFT</b>	Inverse Fast Fourier Transform
<b>LS</b>	Least Squares
<b>ODE</b>	Ordinary Differential Equation
<b>PDE</b>	Partial Differential Equation

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# 1. Fundamentals

## 1.1. Heat Equation

The conduction of heat within a medium can be described using the following partial differential equation (PDE):

$$\frac{\partial u}{\partial t} = \alpha \nabla^2 u \quad (1.1)$$

With  $u$  being a function of space and time and  $\alpha$  being a positive constant. For this paper  $u$  will be defined in terms of one spacial dimension:

$$u := u(x, t) \quad (1.2)$$

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} \quad (1.3)$$

$$x \in \chi \subset \mathbb{R} \quad t \in \tau \subset \mathbb{R} \quad (1.4)$$

$$x_0 \leq x \leq x_n \quad t_0 \leq t \leq t_n \quad (1.5)$$

[1]

In order to not only model the conduction of heat within a medium but also a heating process, a new function  $h : \chi \times \tau \rightarrow \mathbb{R}$  is introduced:

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2} + h(x, t) \quad (1.6)$$

For this paper it is assumed that the initial condition is known:

$$f : \chi \rightarrow \mathbb{R} \quad (1.7)$$

$$u(x, t_0) = f(x) \quad (1.8)$$

### 1.1.1. Solving the Heat Equation using Fourier transform

Applying the Fourier transform (FT) w.r.t  $x$  to 1.6 yields the inhomogeneous ordinary differential equation (ODE):

$$\hat{u} = \mathfrak{F}(u) \quad \hat{h} = \mathfrak{F}(h) \quad (1.9)$$

$$\frac{d}{dt} \hat{u} = -\alpha \omega^2 \hat{u} + \hat{h} \quad (1.10)$$

A solution to 1.10 is given by:

$$\hat{u} = \hat{u}_0 + \hat{u}_p \quad (1.11)$$

Where  $\hat{u}_0$  is the homogeneous solution and  $\hat{u}_p$  is the particular integral. In order to solve this ODE for the particular integral  $\hat{h}$  has to be known. [2] The choice of  $h$  is, except to some restrictions, arbitrary. Therefore an approximate solution to 1.10  $\hat{u}_a$  is obtained by the forward euler scheme:

$$\frac{d}{dt}\hat{u} \approx \frac{\Delta\hat{u}}{\Delta t} \quad (1.12)$$

$$\hat{u}_{t+1} = \hat{u}_t + \Delta t(-\alpha\omega^2\hat{u} + \hat{h}) \quad (1.13)$$

$$\hat{u}_a = [\hat{u}_{t_0}, \dots, \hat{u}_{t_n}] \quad (1.14)$$

In order to apply the euler scheme successfully an initial condition  $\hat{u}_0$  has to be known. This initial condition is obtained by applying the discrete Fourier transform (DFT) to an initial temperature distribution along  $x$ :

$$\hat{u}_0 = \mathfrak{F}(f(x)) \quad (1.15)$$

[3]

The forward euler scheme is used here because it is fairly easy to implement. By applying the inverse discrete Fourier transform (IDFT) to  $\hat{u}_a$  an approximate solution to 1.6 can be obtained. To decrease computing time, the fast Fourier transform (FFT) and inverse fast Fourier transform (IFFT) is used instead of the DFT and IDFT.

## 1.2. Finite Element Method

The finite element method (FEM) is a method to approximate solutions for differential equations (DE) within a certain domain  $\Omega$ . This is done by discretizing the spacial domain. Assume that a DE is given by:

$$m, n \in \mathbb{N} \quad \zeta \in \Omega \subset \mathbb{R} \quad m \geq 1 \quad (1.16)$$

$$\frac{\partial^m y}{\partial \zeta^m} - g(y) = r(\zeta, t) \quad (1.17)$$

It is assumed that  $g$  is a linear function that can also contain partial derivatives of  $y$  w.r.t. time,  $y$  takes the value 0 at the boundary  $\Gamma$  and  $y(\zeta, 0) = f(\zeta)$ . An approximate solution to  $y$  is given by  $\mu$ , which is expressed as a sum of basis functions contained in the set  $\phi$ :

$$\mu(\zeta, t) = \sum_{j=1}^N c_j(t) \phi_j(\zeta) \quad (1.18)$$

The residual is defined as:

$$\mathbf{r} = \frac{\partial^m \mu}{\partial \zeta^m} - g(\mu) - r(\zeta, t) \quad (1.19)$$

Furthermore the residual is required to be orthogonal to all basis functions:

$$\langle \mathbf{r}, \phi_k \rangle = 0 \quad \forall \phi_k \in \phi \quad (1.20)$$

Since the functions in  $\phi$  are known, it is only required to find the coefficients  $c_j(t)$  in 1.18. To find those coefficients 1.20 needs to be expressed as follows:

$$\int_{\Omega} \frac{\partial^m \mu}{\partial \zeta^m} \phi_k d\zeta - \int_{\Omega} g(\mu) \phi_k d\zeta = \int_{\Omega} r(\zeta, t) \phi_k d\zeta \quad \forall \phi_k \in \phi \quad (1.21)$$

If  $\mu$  is substituted with 1.18 the following is obtained:

$$\sum_{j=1}^N \left( \left( \int_{\Omega} \frac{\partial^m \phi_j}{\partial \zeta^m} \phi_k d\zeta \right) c_j(t) - g \left( \left( \int_{\Omega} \phi_k \phi_j d\zeta \right) c_j(t) \right) \right) = \int_{\Omega} r(\zeta, t) \phi_k d\zeta \quad \forall \phi_k \in \phi \quad (1.22)$$

It is also necessary to apply divergence theorem to the first integral term taking into account that  $y$  at  $\Gamma$  is 0. Since  $\zeta$  is one dimensional, the divergence theorem becomes integration by parts:

$$\int_{\Omega} \frac{\partial^m \phi_j}{\partial \zeta^m} \phi_k d\zeta = - \int_{\Omega} \frac{\partial^{m-1} \phi_j}{\partial \zeta^{m-1}} \frac{\partial \phi_k}{\partial \zeta} d\zeta \quad \forall \phi_k \in \phi \quad (1.23)$$

Combining 1.22 and 1.23 yields:

$$-\sum_{j=1}^N \left( \int_{\Omega} \frac{\partial^{m-1} \phi_j}{\partial \zeta^{m-1}} \frac{\partial \phi_k}{\partial \zeta} d\zeta \right) c_j(t) + g \left( \int_{\Omega} \phi_k \phi_j d\zeta \right) c_j(t) = \int_{\Omega} r(\zeta, t) \phi_k d\zeta \quad \forall \phi_k \in \phi \quad (1.24)$$

This formulation leads to a system of ODEs or a system of linear equations that can be solved either analytically or numerically.

### 1.2.1. Solving the Heat Equation using FEM

This formulation of FEM can be applied to 1.6:

$$\Omega = \chi \quad \Gamma = \{x_0, x_n\} \quad (1.25)$$

$$y(\zeta, t) = -u(x, t) \quad g(u) = -\frac{1}{\alpha} \frac{\partial u}{\partial t} \quad (1.26)$$

$$m = 2 \quad r(\zeta, t) = \frac{1}{\alpha} h(x, t) \quad (1.27)$$

$$u(x, 0) = f(x) \quad u(x_0, t) = 0 \quad u(x_n, t) = 0 \quad (1.28)$$

The set of basis functions is defined as a set of piecewise linear functions with constant step size  $\Delta x$ :

$$\phi_j(x) = \begin{cases} (x - x_{j-1})/\Delta x, & x_{j-1} \leq x < x_j \\ (x_{j+1} - x)/\Delta x, & x_j \leq x < x_{j+1} \\ 0, & \text{otherwise} \end{cases} \quad (1.29)$$

[4]

The stepsize  $\Delta x$  is defined by  $\Delta x = \frac{x_n - x_0}{n-1}$ . This results in the following system of ODEs:

$$\sum_{j=1}^N \left( \int_{\chi} \phi_j \phi_k dx \right) \frac{dc_j}{dt} = \alpha \sum_{j=1}^N \left( - \int_{\chi} \frac{d\phi_j}{dx} \frac{d\phi_j}{dx} dx \right) c_j(t) + \int_{\chi} h(x, t) \phi_k dx \quad \forall \phi_k \in \phi \quad (1.30)$$

Using matrix notation this becomes:

$$M^{N \times N}, K^{N \times N} \quad (1.31)$$

$$M \dot{c} = Kc + d \quad (1.32)$$

The matrices  $M$  and  $K$  can be easily computed (Appendix A.1):

$$m_{ij} = \begin{cases} \frac{2\Delta x}{3}, & k = j \\ \frac{\Delta x}{6}, & |k - j| = 1 \\ 0, & \text{otherwise} \end{cases} \quad k_{ij} = \begin{cases} \frac{-2\alpha}{\Delta x}, & k = j \\ \frac{\alpha}{\Delta x}, & |k - j| = 1 \\ 0, & \text{otherwise} \end{cases} \quad (1.33)$$

However it is necessary to approximate  $d$  for each point in time using numerical integration schemes. Furthermore to solve this system of ODEs numerically an initial condition  $c_0$  has to be known. [3]

It can be obtained using a least squares (LS) approach:

$$\sum_{j=1}^N \langle \phi_j, \phi_k \rangle c_j(0) = \langle f, \phi_k \rangle \quad \forall \phi_k \in \phi \quad (1.34)$$

$$M c_0 = F \quad (1.35)$$

$$c_0 = M^{-1} F \quad (1.36)$$

[5]

Observe that by multiplying 1.32 with  $M^{-1}$  (A.2) yields a system of ODEs:

$$\dot{c} = M^{-1} K c + M^{-1} d \quad (1.37)$$

This system of ODEs can be solved using an euler scheme:

$$c_{t+1} = \Delta t M^{-1} (K c_t + d) + c_t \quad (1.38)$$

### Force boundary conditons

Keep in mind that vector  $d$  is time dependent and has to be recomputed for each time step. To force the boudary condition  $u(x, t) = 0 \quad x \in \Gamma$  the first and last entry of any  $c_t$  has to be zero:

$$c_t^1 = 0 \quad c_t^n = 0 \quad \forall t \quad (1.39)$$

Therefore the Matrix  $M^{-1}$  has to be adjusted:

$$0 = \Delta t m (K c + d) \quad (1.40)$$

$$\Rightarrow m = [0, 0, 0, \dots, 0] \quad (1.41)$$

Here  $m$  is the first row vector of  $M^{-1}$  or the last one respectively [3]. Using 1.18 and the computed coefficients  $c$  the function  $u(x, t)$  can be approximated. However this is equivalent to linear interpolation between  $c_n$  and  $c_{n+1}$  (Appendix A.3).

## 1.3. Singular Value Decomposition

The Singular Value Decomposition (SVD) is a matrix factorization with guaranteed existence. It can be used to obtain low rank approximations of a matrix or pseudo inverses for ill posed linear system of equations. It is also related to FT by providing a data specific set of orthogonal bases instead of a generic set of sines and cosines. For this paper the SVD will be used for generating low rank approximations of matrices. [6]

### 1.3.1. Properties

A matrix  $X \in \mathbb{C}^{n \times m}$  can be decomposed in the following way:

$$X = U \Sigma V^* \quad (1.42)$$

Here  $U \in \mathbb{C}^{n \times n}$  and  $V \in \mathbb{C}^{m \times m}$  are unitary matrices and  $\Sigma \in \mathbb{R}^{n \times m}$  is a real valued ordered diagonal matrix. The columns of  $U$  provides a set of orthonormal basis vectors for the column space of  $X$ ,  $V$  contains orthonormal basis vectors for the row space of  $X$ . The matrix  $\Sigma$  assigns a magnitude ('importance') to the product of  $U$  and  $V^*$  [6]. Since  $U$  and  $V$  are unitary they have the following property:

$$U^* U = U U^* = I \quad (1.43)$$

$$V^* V = V V^* = I \quad (1.44)$$

[7]

In case  $n \geq m$  the so called economy SVD can be used to factorize the matrix  $X$ :

$$X = [\hat{U} \quad \hat{U}^\perp] \begin{bmatrix} \hat{\Sigma} \\ 0 \end{bmatrix} V^* = \hat{U} \hat{\Sigma} V^* \quad (1.45)$$

The economy SVD omits rows only containing zeros in  $\Sigma$  and the according columns of  $U$ . Therefore the dimensionality of  $\hat{U}$  and  $\hat{\Sigma}$  is less or equal to the dimensionality of  $U$  and  $\Sigma$ . [6]

### 1.3.2. Hirachy of correlations

As already stated, the matrix  $\Sigma$  assigns a magnitude to  $UV^*$ . This magnitude can be seen as the square of the variance the bases in  $U$  and  $V$  capture. Assume that  $X^* X$  and  $X X^*$  denote a correlation matrix. [6] A correlation matrix is a matrix that stores correlation coefficients between multiple measurements. If  $X$  has the following properties  $X^* X$  and  $X X^*$  are correlation matrices:



1.) The column vectors of  $X$  have to be zero mean:

$$X = [x_1, \dots, x_m] \quad (1.46)$$

$$\frac{1}{n} \sum_{j=1}^n x_{ij} = \mu_i = 0 \quad \forall 1 \leq i \leq m \quad (1.47)$$

2.) The column vectors of  $X$  have to be normalized:

$$\left( \sum_{j=1}^n x_{ij}^2 \right)^{\frac{1}{2}} = \bar{x}_i = 1 \quad \forall 1 \leq i \leq m \quad (1.48)$$

The correlation coefficient between two column vectors of  $X$  is calculated as follows:

$$\text{corr}(x_i, x_{i'}) = \frac{(\sum_{j=1}^n x_{ij} - \bar{x}_i)(\sum_{j=1}^n x_{i'j} - \bar{x}_{i'})}{(\sum_{j=1}^n (x_{ij} - \bar{x}_i)^2)^{\frac{1}{2}} (\sum_{j=1}^n (x_{i'j} - \bar{x}_{i'})^2)^{\frac{1}{2}}} \quad (1.49)$$

[8]

Since all column vectors have zero mean and are normalized this becomes:

$$\text{corr}(x_i, x_{i'}) = \text{cov}(x_i, x_{i'}) = x_i^* x_{i'} \quad (1.50)$$

[9]

This resembles the entries of  $XX^*$  and  $X^*X$ . A vector  $e$  that maximizes the variance of the projections of  $x_i$  onto  $e$  with the restriction  $\|e\| = 1$  are the eigenvectors of the according correlation matrix. The eigenvalue of  $e$  denoted as  $\lambda$  is equivalent to the variance of  $x_i$  projected onto  $e$  [10].

Since  $X$  can be deconstructed using the SVD,  $XX^*$  and  $X^*X$  are equal to:

$$XX^* = U \begin{bmatrix} \hat{\Sigma} \\ 0 \end{bmatrix} V V^* \begin{bmatrix} \hat{\Sigma} & 0 \end{bmatrix} U^* = U \begin{bmatrix} \hat{\Sigma}^2 & 0 \\ 0 & 0 \end{bmatrix} U^* \quad (1.51)$$

$$X^*X = V \begin{bmatrix} \hat{\Sigma} & 0 \end{bmatrix} U^* U \begin{bmatrix} \hat{\Sigma} \\ 0 \end{bmatrix} V^* = V \hat{\Sigma}^2 V^* \quad (1.52)$$

By multiplying  $U$  and  $V$  respectively on the right side 1.51 and 1.52 become:

$$XX^*U = U \begin{bmatrix} \hat{\Sigma}^2 & 0 \\ 0 & 0 \end{bmatrix} \quad (1.53)$$

$$X^*XV = V \hat{\Sigma}^2 \quad (1.54)$$

This shows that  $U$  contains the eigenvectors of the row-wise correlation matrix and  $V$  contains the eigenvectors of the column-wise correlation matrix. The matrix  $\Sigma$  contains the roots of the according eigenvalues and is thereby related to the variance. By ordering  $U$ ,  $\Sigma$  and  $V$  by

the entries of  $\Sigma$  in a descending order the first row of  $U$  and  $V$  contain the most important bases vectors. [6]

### 1.3.3. Low-rank approximation

A usefull property of the SVD is that it can be used to find an hierachy of rank- $r$  approximation for a given matrix  $X$ . An matrix  $\tilde{X}$  that approximates  $X$  is obtained by:

$$\tilde{X} = \arg \min \|X - \tilde{X}\|_F = \tilde{U} \tilde{\Sigma} \tilde{V}^* \quad (1.55)$$

$$s.t. rank(\tilde{X}) = r \quad (1.56)$$

Here  $\tilde{U}$  and  $\tilde{V}$  denote matrices obtained takeing the first  $r$  columns of  $U$  and  $V$ . The matrix  $\tilde{\Sigma}$  is a  $r \times r$  sub-block of  $\Sigma$ . This is alsow known as the Eckard-Young theorem. The variance captured by  $\tilde{X}$  can be calculated in the following way:

$$cumvar_r(\Sigma) = \frac{\sum_{i=1}^r \sigma_i}{trace(\Sigma)} \quad (1.57)$$

$$var(\Sigma) = \frac{diag(\Sigma)}{trace(\Sigma)} \quad (1.58)$$

[6]

### 1.3.4. Example low-rank approximation

As an example suppose there is a matrix  $X \in \mathbb{Z}^{4 \times 4}$ :

$$X = \begin{bmatrix} 3 & 1 & 5 & 5 \\ 4 & -4 & 5 & 0 \\ -4 & -2 & -4 & 3 \\ 5 & 1 & 5 & -4 \end{bmatrix} \quad (1.59)$$

By computing the SVD the matrices  $U$ ,  $\Sigma$  and  $V$  are obtained. Now  $\Sigma$  can be used to calculate the cummulative variance for an rank- $r$  approximation and the variance captured by each basis vector of  $U$  and  $V$ .

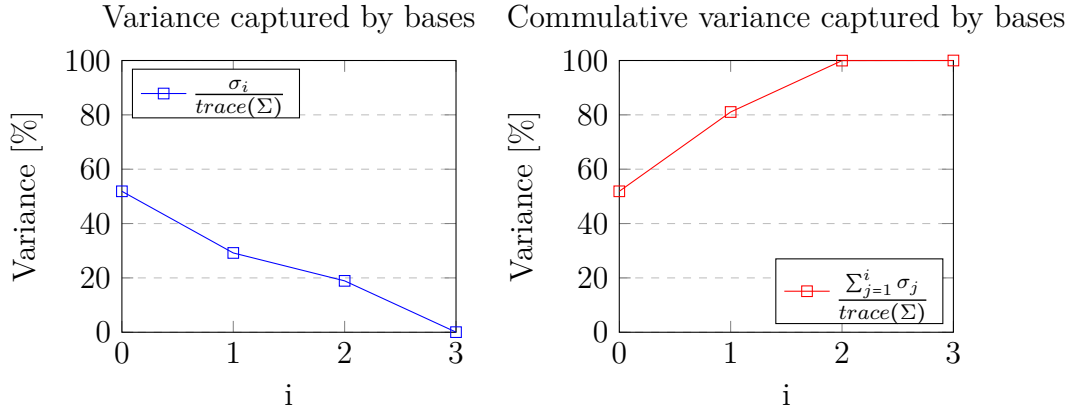


Abbildung 1.1.: Variance and commulative variance captured by each column vectors of  $U$  and  $V$

On 1.3.4 the commulative variance and the variance of each basis vectors is plotted. Here  $X$  can be apprixomated using the first three leading basis vectors. This approximation captures already more than 99% of the variance. The resulting matrix  $\tilde{X}_3$  looks as follows:

$$\tilde{X}_3 = \begin{bmatrix} 4.73 & -0.76 & 5.62 \\ 1.31 & -1.37 & 1.62 \\ -5.10 & -0.60 & 2.34 \end{bmatrix} \quad (1.60)$$

## 2. Model Order Reduction

### 2.1. Introduction

Model Order Reduction (MOR) is a technique to reduce the computational effort of simulate a system using mathematical models. This is done by modeling only the dominant behaviours of those systems [11]. In control theory a system is described by a system of ODEs:

$$\frac{d}{dt}x = Ax + Bu \quad (2.1)$$

$$y = Cx + Du \quad (2.2)$$

This is also called State Space (SS). The State Space

### 3. Implementation

The implementation of the discussed methods for solving the heat equation and for model order reduction was done in Matlab. Matlab was chosen as the programming language because it natively features matrix multiplication which finds heavy use in the previously mentioned methods. The second reason for this selection is that there exist ToolBoxes that already implement certain model order reduction methods such as MORLAB [12] or MOR toolbox [13]. The following figure shows the class diagram of the implementation:

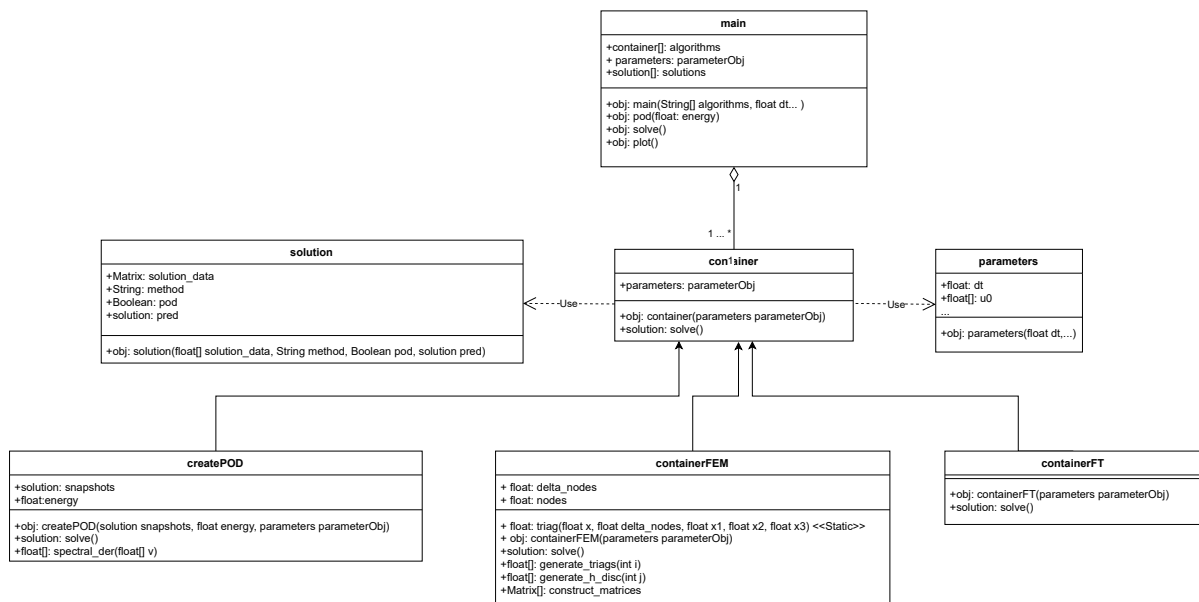


Abbildung 3.1.: Class diagramm of MOR and FEM implementation

### 3.1. Class main

The class main is responsible for generating the finite element solution, model order reduction steps and plotting the results. The process can be seen in the following flow chart:

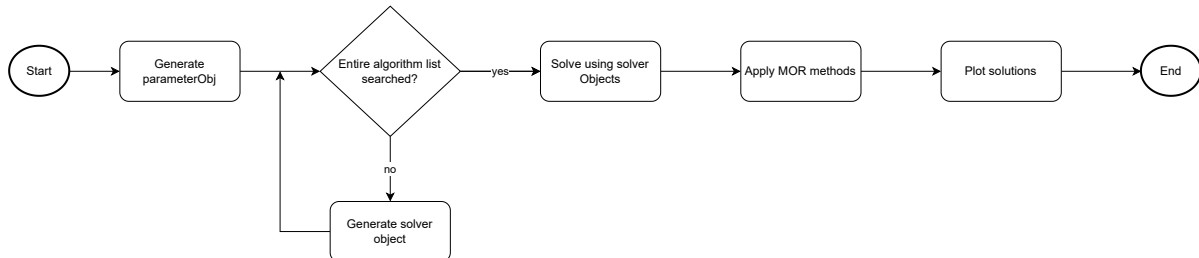


Abbildung 3.2.: Flow chart of main class

The first step is to generate a parameter object. The parameter object stores all parameters in order to increase the transparency and robustness of the program. The second step is to iterate the array of stated algorithms to solve the heat equation. The options are to solve the heat equation using finite element method 1.2 or using fourier transform 1.1. After all solver objects have been generated, the according solutions are being computed. After that, the MOR methods are displayed. The final step is to display the solutions.

### 3.2. Class containerFEM

The class containerFEM is responsible for generating a solution using finite element method. FEM is implemented in the following way:

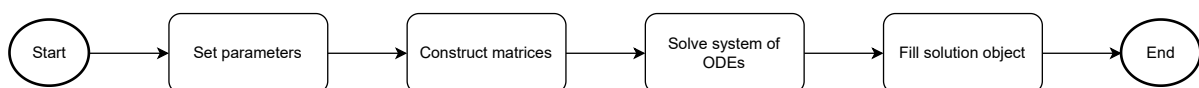


Abbildung 3.3.: Flow chart for FEM class

The first step is to set the parameters. After that the matrices discussed in 1.2 are being constructed. The next step is to solve the resulting system of ODEs and pass the solution to a solution object.

### 3.2.1. Construct Matrices

As defined in 1.33 the matrices  $K$  and  $M$  have to be constructed. Also to compute the initial condition given by  $u_0$   $F$  has to be known 1.35. This is done by the following method:

---

**Algorithmus 1** Construct matrices  $K$ ,  $M$  and  $F$ 

---

```
1:  $ii \leftarrow \frac{2}{3}\Delta nodes$ 
2:  $ij \leftarrow \frac{1}{6}\Delta nodes$ 
3:  $F \leftarrow \text{zeros}(nodes, 1)$ 
4:  $K \leftarrow \text{zeros}(nodes)$ 
5:  $M \leftarrow \text{zeros}(nodes)$ 
6: for  $i = 1$  to  $nodes$  do
7:    $F(i) \leftarrow \text{trapz}(\phi_i \cdot u_0)$ 
8: end for
9: for  $i = 1$  to  $nodes$  do
10:    $K(i, i) \leftarrow \frac{-2}{\Delta nodes}$ 
11:    $M(i, i) \leftarrow ii$ 
12:   if  $i - 1 > 1$  then
13:      $K(i, i - 1) \leftarrow \frac{1}{\Delta nodes}$ 
14:      $M(i, i - 1) \leftarrow ij$ 
15:   end if
16:   if  $i + 1 < nodes + 1$  then
17:      $K(i, i + 1) \leftarrow \frac{1}{\Delta nodes}$ 
18:      $M(i, i + 1) \leftarrow ij$ 
19:   end if
20: end for
21: return  $[F, K, M]$ 
```

---

### 3.2.2. Compute vector $d(t)$

As discussed in 1.2 vector  $d$  has to be computed for each time step:

---

**Algorithmus 2** Construct vector  $d$ 

---

```
1:  $d \leftarrow \text{zeros}(nodes, 1)$ 
2: for  $i = 1$  to  $nodes$  do
3:    $d(i) \leftarrow \text{trapz}(\phi_i \cdot h(x, t_0))$ 
4: end for
5: return  $d$ 
```

---

The entries of vector  $d$  become the integral of the product of a basisfunction and  $h$  evaluated at timestep  $t_0$ . This timestep is a argument of that method.

### 3.2.3. Solve System of ODEs

The most important step in the process of generating a solution is to solve the system of ordinary differential equations that FEM yields:

---

**Algorithmus 3** Solve system of ODEs using euler's scheme

---

```
1:  $[F, K, M] \leftarrow \text{construct\_matrices}()$ 
2:  $C \leftarrow \text{zeros}(\text{nodes}, n\_time\_steps)$ 
3:  $c_0 \leftarrow M^{-1}F$ 
4:  $C(:, 1) \leftarrow c_0$ 
5:  $M(1, :) \leftarrow [0, \dots, 0]$ 
6:  $M(\text{end}, :) \leftarrow [0, \dots, 0]$ 
7:  $N \leftarrow M^{-1}K$ 
8: for  $t = 2$  to  $n\_time\_steps$  do
9:    $d \leftarrow \text{generate\_h\_disc}(t)$ 
10:   $c_n \leftarrow \Delta t N c_0 + M^{-1}h + c_0$ 
11:   $c_0 \leftarrow c_n$ 
12:   $C(:, t) \leftarrow c_n$ 
13: end for
14:  $S \leftarrow []$ 
15: for  $t = 1$  to  $n\_time\_steps$  do
16:   $c \leftarrow C(:, t)$ 
17:   $\text{interpol} \leftarrow \text{interp1}(\text{linspace}(0, L, \text{nodes}), c, X)$ 
18:   $S(:, t) \leftarrow \text{interpol}$ 
19: end for
20: return  $\text{solution}(S, "FEM", 0, 0)$ 
```

---

In the first line the matrices  $F$ ,  $K$  and  $M$  are retrieved. After that the initial vector of coefficients  $c_0$  is computed using LS 1.36 in line three. The next two following lines force the boundary conditions as stated in 1.41. In the lines 8 to 13 1.38 is implemented. In the last step the coefficients are interpolated in spatial direction to fit the given domain  $X$  and stored in a solution object.



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# A. Appendix

## A.1. Deriving matrices for FEM using piecewise linear functions

The so called triangle function is defined as follows:

$$\phi_j(x) = \begin{cases} (x - x_{j-1})/\Delta x, & x_{j-1} \leq x < x_j \\ (x_{j+1} - x)/\Delta x, & x_j \leq x < x_{j+1} \\ 0, & \text{otherwise} \end{cases} \quad (\text{A.1})$$

[4] The following integrals have to be evaluated:

$$\int_{\chi} \phi_j \phi_k dx \quad \forall \phi_k \in \phi \quad (\text{A.2})$$

$$- \int_{\chi} \frac{d\phi_j}{dx} \frac{d\phi_k}{dx} dx \quad \forall \phi_k \in \phi \quad (\text{A.3})$$

With  $\chi \subset \mathbb{R}$ . Note that the product of two functions  $\phi_j$  and  $\phi_k$  and their derivatives is only under two conditions not zero:

1.  $k = j$

Considering this case the integral A.2 becomes:

$$\int_{x_{j-1}}^{x_j} \phi_j^2 dx + \int_{x_j}^{x_{j+1}} \phi_j^2 dx \quad (\text{A.4})$$

Because of symmetry only one of the above integrals have to computed:

$$2 \int_{x_{j-1}}^{x_j} \phi_j^2 dx \quad (\text{A.5})$$

$$= \frac{2}{\Delta x^2} \int_{x_{j-1}}^{x_j} (x - x_{j-1})^2 dx \quad (\text{A.6})$$

$$\frac{2}{3\Delta x^2} [(x - x_{j-1})^3]_{x_{j-1}}^{x_j} = \frac{2}{3\Delta x^2} \Delta x^3 = \frac{2}{3} \Delta x \quad (\text{A.7})$$

Integral A.3 for  $i = j$  taking symmetry into account becomes:

$$- \int_{x_{j-1}}^{x_{j+1}} \left( \frac{d\phi_j}{dx} \right)^2 dx = - \frac{1}{\Delta x^2} \int_{x_{j-1}}^{x_{j+1}} 1 dx \quad (\text{A.8})$$

$$= - \frac{1}{\Delta x^2} [x]_{x_{j-1}}^{x_{j+1}} = - \frac{2}{\Delta x} \quad (\text{A.9})$$

2.  $|j - k| = 1$  A.2 becomes:

$$\frac{1}{\Delta x^2} \int_{x_j}^{x_{j+1}} (x - x_j)(x_{j+1} - x) dx \quad (\text{A.10})$$

$$= \left[ \frac{1}{2} x^2 x_{j+1} - \frac{1}{3} x^3 - x x_{j+1} x_j + \frac{1}{2} x^2 x_j \right]_{x_j}^{x_{j+1}} = \frac{1}{6 \Delta x^2} \Delta x^3 = \frac{1}{6} \Delta x \quad (\text{A.11})$$

Finally A.3 has to be evaluated for this condition:

$$- \int_{x_j}^{x_{j+1}} \frac{d\phi_j}{dx} \frac{d\phi_{j+1}}{dx} dx = \frac{1}{\Delta x^2} \int_{x_j}^{x_{j+1}} 1 dx = \frac{1}{\Delta x^2} [x]_{x_j}^{x_{j+1}} = \frac{1}{\Delta x} \quad (\text{A.12})$$

## A.2. Proof that matrix $M$ is invertible

Let  $M_n$  be a matrix with  $M_n \in \mathbb{R}^{n \times n}$  given by:

$$m_{ij} = \begin{cases} a, & k = j \\ b, & |k - j| = 1 \\ 0, & otherwise \end{cases} \quad (\text{A.13})$$

It's determinant is given by the Laplace expansion:

$$\det(M_n) = \sum_{j=1}^n (-1)^{i+j} a_{ij} N_{ij} \quad \forall i \quad (\text{A.14})$$

$N_{ij}$  is the determinant of the matrix  $M'$  that is obtained by removing the  $i^{th}$  row and  $j^{th}$  column of  $M_n$ . This expression can be simplified using the definition of  $m_{ij}$ :

$$\det(M_n) = aN_{11} - bN_{12} \quad (\text{A.15})$$

$N_{11}$  is equivalent to  $\det(M_{n-1})$ , since the indices of rows and columns of  $M'$  are in consecutive order and  $M'$  is a  $n-1 \times n-1$  matrix :

$$N_{11} = \det(M') \quad (\text{A.16})$$

$$M' = \begin{bmatrix} m_{22} & \dots & m_{2n} \\ \vdots & \ddots & \vdots \\ m_{n2} & \dots & m_{nn} \end{bmatrix} \quad (\text{A.17})$$

$N_{12}$  can be obtained by calculating the determinant of  $M'$  using the Laplace expansion:

$$M' = \begin{bmatrix} m_{21} & m_{23} & \dots & m_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ m_{n1} & m_{n3} & \dots & m_{nn} \end{bmatrix} \quad (\text{A.18})$$

$$\det(M') = m_{21} \cdot \det(M'') \quad (\text{A.19})$$

$$M'' = \begin{bmatrix} m_{33} & \dots & m_{3n} \\ \vdots & \ddots & \vdots \\ m_{n3} & \dots & m_{nn} \end{bmatrix} \quad (\text{A.20})$$

In A.19 only the stated term has to be evaluated since all entries of the first column of the second submatrix are zero. Therefore the determinant is zero. The row and column indices of  $M''$  are in consecutive order and it is a  $n-2 \times n-2$  matrix. Therefore  $M''$  is equivalent to  $M_{n-2}$ . A.15 becomes:

$$\det(M_n) = a \cdot \det(M_{n-1}) - b^2 \cdot \det(M_{n-2}) \quad (\text{A.21})$$

Furthermore this implies  $\det(M_0) = 1$ :

$$\det(M_2) = a^2 - b^2 = a \cdot \det(M_1) - b^2 \cdot 1 \quad (\text{A.22})$$

$$\Rightarrow \det(M_0) = 1 \quad (\text{A.23})$$

Using the definition of 1.33 and 1.2.1 this can be seen as the following sequence:

$$a_0 = 1, \quad a_1 = \frac{2\Delta x}{3} \quad (\text{A.24})$$

$$a_{n+1} = \frac{2\Delta x}{3} \cdot a_n - \frac{\Delta x^2}{36} \cdot a_{n-1} \quad (\text{A.25})$$

As described here [14] a recursive sequence converges if it is monotone and has a limit. A proof by induction shows that this sequence is monotone for  $n \geq 1$ .

Base case:

$$a_2 = \left(\frac{2\Delta x}{3}\right)^2 - \frac{\Delta x^2}{36} = \Delta x^2 \left(\frac{4}{9} - \frac{1}{36}\right) < \frac{2\Delta x}{3} = a_1 \quad (\text{A.26})$$

Induction step: Assuming that  $a_k < a_{k-1}$  holds,  $a_{k+1} < a_k$  also holds:

$$a_{k+1} = \frac{2\Delta x}{3} \cdot a_k - \frac{\Delta x^2}{36} \cdot a_{k-1} < \frac{2\Delta x}{3} \cdot a_{k-1} - \frac{\Delta x^2}{36} \cdot a_{k-2} = a_k \quad (\text{A.27})$$

The limit of this sequence is as follows:

$$\alpha = \lim_{n \rightarrow \infty} a_{n+1} = \lim_{n \rightarrow \infty} \Delta x \cdot \frac{2}{3} \cdot \lim_{n \rightarrow \infty} a_n - \lim_{n \rightarrow \infty} \Delta x^2 \cdot \frac{1}{36} \cdot \lim_{n \rightarrow \infty} a_{n-1} = 0 \cdot \alpha - 0 \cdot \alpha = 0 \quad (\text{A.28})$$

Since this series is monotone and converges to zero as  $n$  goes to infinity, there is no  $n \in \mathbb{N}$  for which  $a_n = 0$ . Therefore the determinant of the matrix  $M$  defined in 1.33 is not zero and  $M$  is invertible.

### A.3. Equivalence of picewise linear polynomials and linear interpolation

A picewise linear polynomial in the form of:

$$u(x, t) = \sum_{j=1}^N c_j(t) \phi_j(x) \quad (\text{A.29})$$

With  $\phi_j$  being defined as A.1 and  $c_j : \mathbb{R} \rightarrow \mathbb{R}$  is equivalent to linear interpolation with respect to  $x$ :

$$\hat{u}(x, t) = u_j + \frac{(u_{j+1} - u_j)(x - x_j)}{x_{j+1} - x_j} \quad (\text{A.30})$$

for  $x_j < x < x_{j+1}$  [15]. This can be shown by evaluating  $u(x, t)$  between two neighbouring  $\phi$  and  $x_j < x < x_{j+1}$ :

$$u(x, t) = \phi_j(x) c_j(t) + \phi_{j+1}(x) c_{j+1}(t) \quad (\text{A.31})$$

$$= \frac{x_{j+1} - x}{\Delta x} c_j(t) + \frac{x - x_j}{\Delta x} c_{j+1}(t) \quad (\text{A.32})$$

$$= \frac{x_{j+1} - x}{\Delta x} u_j + \frac{x - x_j}{\Delta x} u_{j+1} \quad (\text{A.33})$$

$$= \frac{(x_{j+1} u_j - x u_j) + (x u_{j+1} - x_j u_{j+1})}{\Delta x} \quad (\text{A.34})$$

$$= \frac{(u_{j+1} - u_j)x + x_{j+1} u_j - x_j u_{j+1}}{\Delta x} \quad (\text{A.35})$$

$$= \frac{(u_{j+1} - u_j)x + x_j u_j + \Delta x u_j - x_j u_{j+1}}{\Delta x} \quad (\text{A.36})$$

$$= u_j + \frac{(u_{j+1} - u_j)x - x_j(u_{j+1} - u_j)}{\Delta x} \quad (\text{A.37})$$

$$= u_j + \frac{(u_{j+1} - u_j)(x - x_j)}{x_{j+1} - x_j} \quad (\text{A.38})$$